CONTENTS

AM1 paramters for phosphorus
M.J.S. Dewar and C. Jie (Austin, TX, U.S.A.) 1
Categories in chemistry and chemical computers
L. Schulz (Poznan, Poland) 15
Modelling of angular dependence of superexchange: application to copper(II) dimers
M. Atanasov and S. Angelov (Sofia, Bulgaria) and I. Mayer (Budapest, Hungary) 23
On the vibrational transition selection rules for the centrosymmetric hydrogen-bonded dimeric systems
H.T. Flakus (Katowice, Poland) 35
AM1 study of hydrogen bonded complexes of water
O.N. Ventura, E.L. Coitiño, A. Lledós and J. Bertrán (Montevideo, Uruguay) 55
An ab initio structural investigation of 1,3-butadiene, isoprene and 2,3-dimethyl-1,3-butadiene rotamers
Ch.W. Bock (Marcus Hook, PA, U.S.A.) and Yu.N. Panchenko (Moscow, U.S.S.R.) 69
The periodic system of chemical elements: old and new developments
M. Kibler (Villeurbanne, France) 83
A computational study of the structures and electrostatic potentials of some azines and nitroazines
J.S. Murray, J.M. Seminario and P. Politzer (New Orleans, LA, U.S.A.) 95
On the absence of isotope effects in high-T_c superconductors and the role of (Cooper) pairs in bonding
G. van Hooydonk (Gent, Belgium) 109
A theoretical study of the influence of noradrenaline ring fluorination on its adrenergic activity
T.J. Mitchell, M.S. Tute and G.A. Webb (Surrey, Gt. Britain) 115
On the relation between electron density, molecular structure and intramolecular forces in neutral and protonated formaldehyde and halogen substituted analogs
Z. Karpas, A.T. Hagler, F. Sussman and P.S. Stern (Rehovot, Israel) 123
Free electron PMO: *F*-omega model with variable electronegativity and self-interaction correction: application to ionic reaction intermediates
L. von Szentpály (Guanajuato, Mexico) 139
Furan revisited: when to avoid ab initio studies on crystal structures
C.L. Verlinde and C.J. De Ranter (Leuven, Belgium) 161
Strain in heterocycles
P. Siddarth and M.S. Gopinathan (Madras, India) 169
Ab initio investigations of symmetric rotor models for small trifluoromethyl substituted molecules
A.H. Lowrey (Washington, DC, U.S.A.) 177
Ab initio study of internal rotation of the vinylphosphine molecule: $H_2C{=}CH{-}PH_2$
M.B. Zuev and V.A. Naumov (Kazan, U.S.S.R.) 191
Novel [4+2] cycloaddition reactions of ketenimines: a semiempirical molecular orbital study
W.M.F. Fabian and G. Kollenz (Graz, Austria) 199
Calculation of **g**-values of free radicals by finite perturbation theory
M. Ishii, K. Morihashi and O. Kikuchi (Tsukuba, Japan) 209
Theoretical calculations on the 1:1 complexes of N-aromatics with water
G. Alagona and C. Ghio (Pisa, Italy) and P. Nagy (Budapest, Hungary) 219
Theoretical study of B_2H_n (with $n=2$ to 6): molecules and related positive ions
M. Sana and G. Leroy (Louvain-la-Neuve, Belgium) and Ch. Henriet (Paris, France) 233

Heats of formation of some energetic compounds containing NO_2 and/or NF_2 groups
G. Leroy, M. Sana, C. Wilante and D. Peeters (Louvain-la-Neuve, Belgium) and S. Bourasseau (Châtillon, France) 251
The effect of geometerical relaxation on the rotational barrier of ethane
E. Honegger (Bern, Switzerland) 261
Ab initio studies of structural features not easily amenable to experiment. Part 65. Ab initio molecular structures of glyoxylic, pyruvic, and propiolic acid, and comparison with microwave data
C. van Alsenoy (Wilrijk, Belgium), L. Schafer, K. Siam and J.D. Ewbank (Fayetteville, AR, U.S.A.) 271
Remarks on Kekuléan and non-Kekuléan benzenoid hydrocarbons
R.-Q. Sheng (Shanghai, China), S.J. Cyvin and I. Gutman (Trondheim, Norway) 285
Theoretical investigation of the hindered amine photostabilising mechanism
A. Bolotin, P. Pipiraite and A. Ružiene (Vilnius, U.S.S.R.) 291
AM1 outer valence Green's function ionization energies of the azoles
D. Danovich, V. Zakrzewski and E. Domnina (Irkutsk, U.S.S.R.) 297
Conformation of *N*-acetyl-L-pro-D-ala-*N'*-methyl tripeptide: empirical, semi-empirical MO and ab initio MO calculations
J. Mavri, F. Avbelj and D. Hadži (Ljubljana, Yugoslavia) 307
Ab initio study of the structures and vibrational frequencies of CH_3SiF_3, $[CH_3SiF_4]^-$ and $[CH_3SiF_5]^{2-}$
S. Sakai and M. Imoto (Suita, Japan) 317
Conformations and electronic structure of dithiin, 1,4-dithiino[2,3-*C*:6,5-*C'*]diisothiazole and its derivatives
G. Buemi and C. Gandolfo (Catania, Italy) 325
Ab initio force constants: a cautionary tale concerning nitrogen oxides
C.J. Marsden and B.J. Smith (Parkville, Vic., Australia) 337
On the interconnection of metal–metal bonding in dimers and solid resistivity, magnetic susceptibility, and normal superconductivity
N.D. Epiotis (Seattle, WA, U.S.A.) 359

Author index 395

Subject index 396